

Modeling of Long Term Carbon Sequestration in Different Coal Seams

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Abstract

A long term projection of CO₂ transport and possible escape from deep coal seams is an important problem associated with CO₂ sequestration. Many factors can affect the process of CO₂ transport, such as bounding layers permeabilities, porosities, fracture densities, etc. In this study a computer simulation was conducted with a purpose of predicting CO₂ transport in a multi-layer environment of typical unmineable coal seams. Typical characteristics from the database of three coal basins were used in the simulations. TOUGH2 simulator was used to predict CO₂ transport. A four layer of sand-shale-coal-shale was considered with the overlying and underlying medium to be the shales.

Fracture zones are the main problem and might present local escape points. Locating faults and fracture zones is one of the objectives of the geophysical characterization and monitoring efforts. However, a lot of this will be site dependent. In this study different scenarios including tight seal versus leaky seal were considered. In a tight-seal case, the results show a slow but non-negligible spreading of CO₂ in the layer of coal, and after a sufficiently long time some of them also spreading to the shale layers. However, in the tight-seal case no significant penetration was predicted for up to 100 years. On the other hand, in the loose seal case, the speed of the spread of CO₂ to shale and sand layers was much faster, showing a considerable leakage after 50 years. Thus, computer simulations can help to select suitable reservoirs for CO₂ sequestration.

1 Introduction

CO₂ is a main source of greenhouse gas, which pollutes the atmosphere, CO₂ sequestration is one solution to the problem, which may help to bring down the atmospheric pollution. As shown in recent surveys [1], about one third of all CO₂ emissions comes from the fossil fuels, used for generating electricity and some industrial process such as oil refineries, production of cement, iron and steel, with each plant emitting several million tonnes of CO₂ annually. Just this injection of enormous CO₂ amounts into the environment results in a series of global problems as warming of the climate and deforestation, caused by acid rain. CO₂ capture and sequestration may help to slow down this process and avoid further pollution of the natural environment. In addition to that it may bring other benefits, such as the coal bed methane recovery, enhanced oil recovery and enhanced gas recovery. Whatever the options of CO₂ sequestration in different basins or reservoirs, the crucial problem is to find safe and secure geological reservoirs to store the gas and make sure that no leakage will develop over a long time.

At present, there are three options of CO₂ sequestration. One is to inject the CO₂ into a deep coal bed, where it will be absorbed by the coal, typically displacing methane as a result. Typically the residual coal bed methane can also be recovered in this operation. Another option is to pump the CO₂ into saline formations where CO₂ dissolves into the ambient fluid. The last option is to store the CO₂ into the oil or natural gas reservoirs where it will replace the oil and gas as they are being recovered [1]. As the reference shows, there are some potential reservoirs for this type of operation. However, a more comprehensive study still needs to be done on the feasibility of CO₂ sequestration [2]. One of the most important things is the consideration of safety and longevity of CO₂ underground storage whatever the type of options and reservoirs. In particular, an important question is how effectively would the CO₂ be sealed in reservoirs to avoid leaking. Thus, the key problem is to find the appropriate geological reservoirs to realize the storage for CO₂. For this purpose, different geological reservoirs were investigated in this study. Some of the typical parameters were used to simulate various scenarios of CO₂ sequestration with the purpose of analyzing long term containment characteristics of the reservoirs.

2 Method

In this study, the TOUGH2 simulator [3] was adopted to predict CO2 transport in the porous media of the seams and surrounding layers. TOUGH2 is widely used, as a numerical simulated tool, to solve some groundwater problems such as geothermal reservoirs, nuclear waste isolation and other related problems [4]. Basically TOUGH2 solves mass and heat transfer problems for multicomponent and multiphase fluids in two or three dimensional porous media based on the mass and energy conservation equations by the finite volume method [5]. The iteration procedure is based on the Newton linear equation solution [6] of the basic mass and energy balance equations:

$$\frac{d}{dt} \int_V M^i dV = \int_{\Gamma} (\vec{F}^i \cdot \vec{n}) d\Gamma + \int_V q^i dV \quad (1)$$

where the arbitrary subdomain V of the flow is enclosed by the boundary surface Γ , \vec{F}^i represents the mass or energy flux of specie i , while q denotes sinks and sources, and \vec{n} is the normal vector which points into V on surface $d\Gamma$. M^i is the specie concentration or energy density with $i = 1, \dots, CN$ denoting the CN components, such as water, air, H_2 etc.

$$M^i = \phi \sum_{\beta} S_{\beta} \rho_{\beta} X_{\beta}^i \quad (2)$$

Here, ϕ is the porosity, β is the index of the liquid/solid phase, S_{β} is the saturation, ρ_{β} is the density, and X_{β}^i is the mass fraction of the component i present in phase β .

Advection mass flux is computed as the sum over the phases as follows:

$$F_{adv}^i = \sum_{\beta} X_{\beta}^i F_{\beta} \quad (3)$$

For each phase the F_{β} is defined as:

$$F_{\beta} = \rho_{\beta} u_{\beta} = -k \frac{k_{r\beta}}{\mu_{\beta}} (\nabla P_{\beta} - \rho_{\beta} g) \quad (4)$$

Where, u_{β} is the Darcy velocity, k is absolute permeability, $k_{r\beta}$ is relative permeability of phase β . μ_{β} is viscosity.

Also, the heat flux includes conductive and convective components:

$$F^{CN+1} = \lambda \nabla T + \sum_{\beta} h_{\beta} F_{\beta} \quad (5)$$

where λ is the thermal conductivity, and h_{β} is specific enthalpy in phase β . For Darcy flows, the diffusion and hydrodynamic dispersion were considered as well:

$$F_k = - \sum_{\beta} \rho_{\beta} \bar{D}_{\beta} \nabla X_{\beta}^i \quad (6)$$

The hydrodynamic dispersion tensor, \bar{D}_{β} , is defined as:

$$\bar{D}_{\beta} = D_{\beta,T}^i \bar{I} + \frac{(D_{\beta,L}^i - D_{\beta,T}^i)}{u_{\beta}^2} u_{\beta} u_{\beta} \quad (7)$$

where

$$\begin{aligned} D_{\beta,L}^i &= \phi \tau_0 \tau_{\beta} d_{\beta}^i + \alpha_{\beta,L} u_{\beta} \\ D_{\beta,T}^i &= \phi \tau_0 \tau_{\beta} d_{\beta}^i + \alpha_{\beta,T} u_{\beta} \end{aligned}$$

and d_{β}^i is the molecular diffusion coefficient for component i in phase β , $\tau_0 \tau_{\beta}$ is the tortuosity which includes a porous medium dependent factor τ_0 and a coefficient that depends on phase saturation S_{β} , $\tau_{\beta} = \tau_{\beta}(S_{\beta})$. α_L , α_T are the longitudinal and transverse dispersivities. If the mass flux is due to molecular diffusion alone, then $\alpha_L = \alpha_T = 0$. The diffusive flux of component i in phase β is given by:

$$f_{\beta}^i = -\phi \tau_0 \tau_{\beta} \rho_{\beta} d_{\beta}^i \nabla X_{\beta}^i \quad (8)$$

Applying the Gauss divergence theorem to equation (1) becomes the PDE as:

$$\frac{\partial M^i}{\partial t} = -\text{div} F^i + q^i \quad (9)$$

This continuum equation is discretized in space and time by integral finite volume approximations [5, 7, 8].

In this study, three typical different geological reservoirs of coal bed basin were selected and simulated. All of the simulations were performed on two grids: 25X25X25 and 25X50X50. The diffusive transport of underground CO₂ was recorded at several time instances: 1, 5, 20, 50, and 100 years. The results computed on different grids were compared and analyzed.

Table 1: Reservoir Parameters

Parameter	San Juan	Appalachian	Powder River
Average Depth, ft	3250	1500	800
Gross Interval, ft	200	1200	60
Net Coal Thickness, ft	45	13	60
Zones Completed	1-3	8-13	1
Reservoirs Pressure, phi	1300	500	340
Gas Content, scf/ton	450	300	75
Ash Content, %	15	12	10
Moisture Content, %	2	2	20
Permeability, md	5-50	1-10	20-400+
Porosity, %	0	1	2
Initial Water Saturation, %	100	100	100
Well Spacing, ac/well	320	80	80
GIP per well, Bscf	9.5	0.5	0.4

Table 2: San Juan Basin. Domain size: $960 \times 960 \times 960 \text{ m}^3$

Layer	Thickness (m)	Density (kg/m^3)
Sand	317	2550
Top Shale	317	2100
Coal	39	1380
Bottom Shale	317	2100

3 Results

The parameters of the three typical coal basins were considered: San-Juan, Appalachian, and Powder River, which were taken from the GASIS database [9], and correlated with other sources [10, 11, 12, 13]. The excerpts from the data are listed in the Tables 1 - 4.

According to the information sources available to us [13], the plan for the CO₂ sequestration intermediate scale pilot project was to inject 750,000 tons per year. We conducted the simulation considering a 12 point injection, which for the above total injection gives an injection rate of about 2 kg/sec per injection point. The results of transient simulations executed with TOUGH2 simulator are shown in Figures 1, 2, 3:

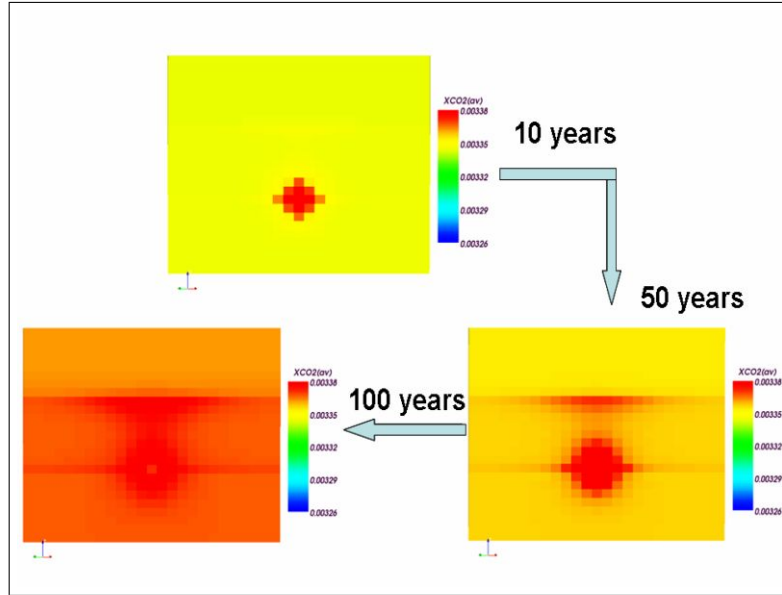


Figure 1: San-Juan Basin: vertical cross-sections of CO₂ concentration with the rate of injection 2.0 kg/second

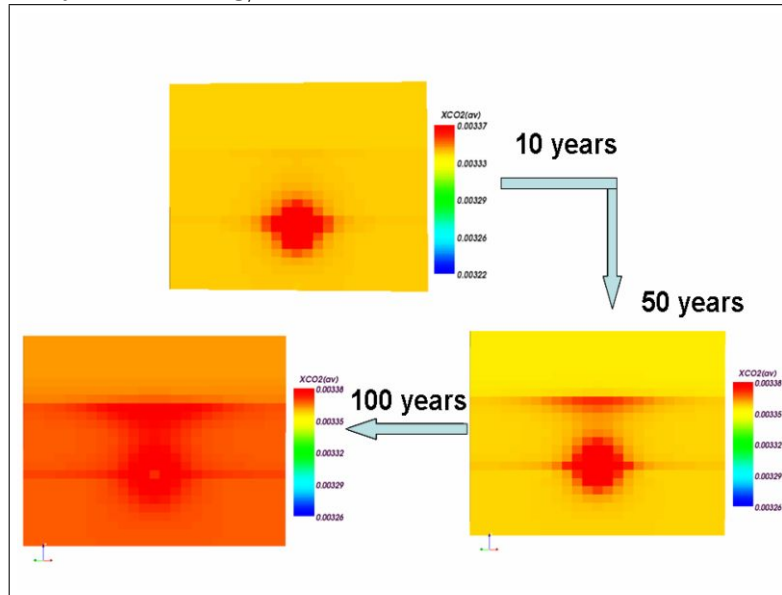


Figure 2: Appalachian Basin: vertical cross-sections of CO₂ concentration with the rate of injection 2.0 kg/second

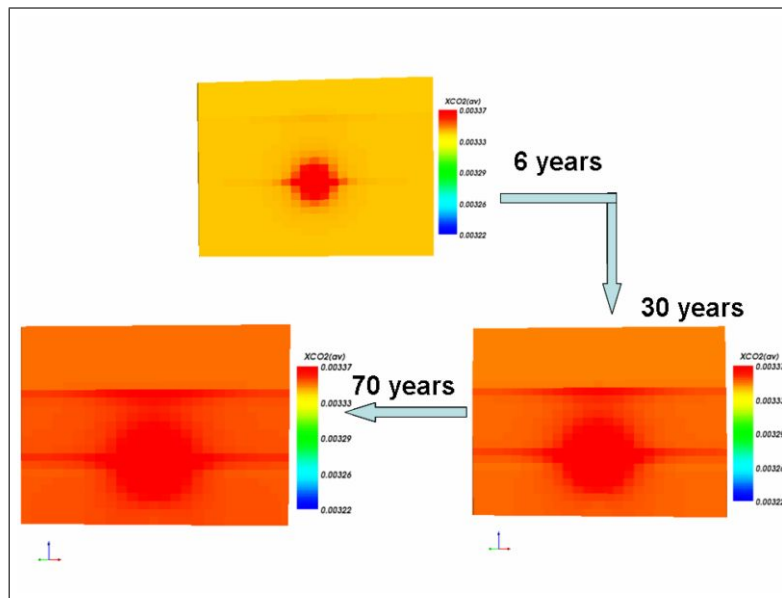


Figure 3: Powder River: vertical cross-sections of CO₂ concentration with the rate of injection 2.0 kg/second

Table 3: Appalachian Basin. Domain size: $457 \times 457 \times 457 \text{ m}^3$.

Layer	Thickness (m)	Density (kg/m^3)
Sand	91	2650
Top Shale	165	2200
Coal	18	1350
Bottom Shale	183	2200

Table 4: Powder River Basin. Domain size: $243 \times 243 \times 243 \text{ m}^3$.

Layer	Thickness (m)	Density (kg/m^3)
Sand	76	2600
Top Shale	78	2010
Coal	19	1280
Bottom Shale	68	2010

The simulations performed on finer grids generally were in a good agreement with the coarse grid results. Figure 4 shows the snapshot of the CO₂ distribution for the San Juan basin.

The analysis of the effects of possible lower higher permeability seals produces different CO₂ distributions in shale layers, as shown in Fig.5. However, as long as the permeability in the top layer stays the same this does not significantly affect the CO₂ containment in the reservoir.

The results can be summarized as follows. For San Juan coal bed reservoir, with the geological layers distribution as shale, sandstone, coal and shale, the expected CO₂ containment within the coal layer is about 50 years. And for the Central Appalachian Coal Basin, the expected containment is 20 years, depending on the composition of layers and layout. For the Powder River Basin there was no considerable leakage of CO₂ after 50 years. The conclusion is that the San Juan and Powder River basins appear to be suitable for CO₂ sequestration. Nevertheless a more thorough researches to confirm these findings will be needed.

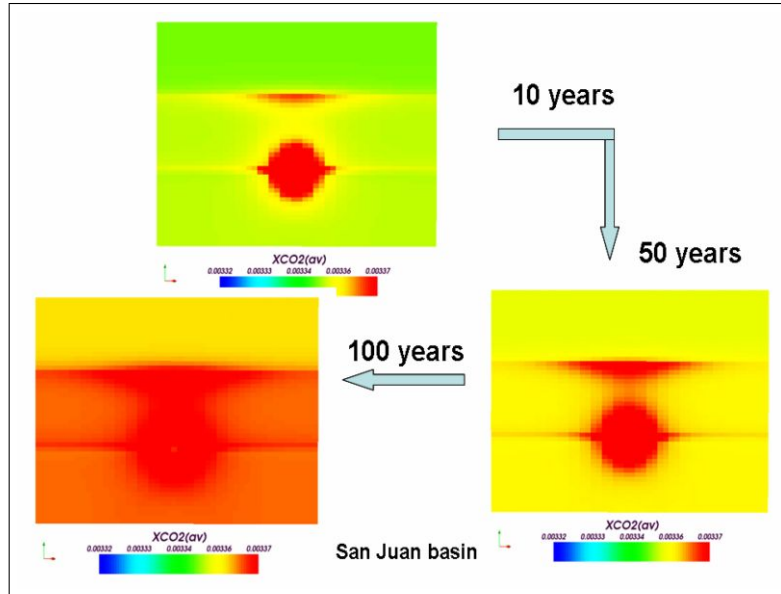


Figure 4: San-Juan Basin: vertical cross-section of CO₂ concentration with the rate of injection 2.0 kg/second on a finer grid

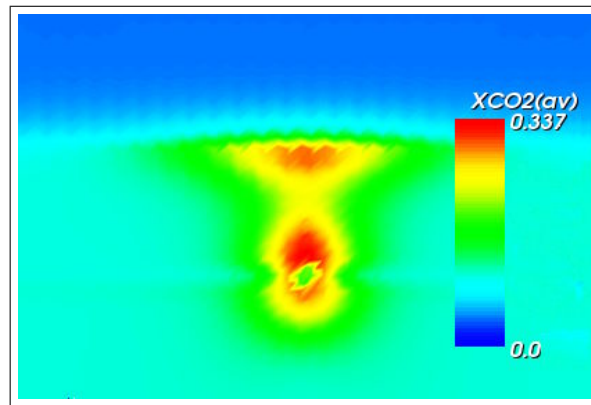


Figure 5: The vertical CO₂ concentration after 50 years with a higher permeability in the shale layer

4 Conclusions and Future Work

Computer simulations of CO₂ sequestration in geological formations can offer valuable long-term forecasts of capacity, durability and containment characteristics of different reservoirs. In fact they seem to be the only way to analyze the feasibility and long-term impact of geological CO₂ sequestration operations. However, a large number of parameters, which need to be considered, and the lack of accurate data on some of the parameters, can create big uncertainties in forecasts. It is still possible to use computer simulations under uncertainty in a sense of probabilistic risk assessments. In particular, playing out different scenarios may help to identify the limits of what can be expected and assist in the analysis of certain extreme cases.

This study showed that using the available data it is possible to conduct a relative analysis of different coal basins on their suitability for CO₂ sequestration. Currently only the two phase CO₂/H₂O system was considered with liquid and gas phases. An interesting case would be to consider coal-bed methane recovery enhanced by CO₂ injection. This analysis will help to identify economic benefits and possible sustainability of CO₂ sequestration operations. In this case a three component CO₂/H₂O/CH₄ model should be used, which will be the subject of the future study.

Further work should be done with the improved modeling capabilities, so as to predict the CO₂ transport in the localities of fracture zones, which might present the local escape points.

Acknowledgments

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